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Supporting Information

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Supporting information for the manuscript "The ReaxFF Monte Carlo Reactive Dynamics Method for Predicting Atomistic Structures of Disordered Ceramics: Application to the Mo_3VO_x Catalyst" by Kimberly Chenoweth, Adri C.T. van Duin, and William A. Goddard, III.

Computational Details:

The Monte Carlo simulations were run for 500,000 steps with a Monte-Carlo swap temperature of 5000K and a displacement temperature of 500K with a 0.1Å step size for displacements until energy convergence was achieved for each starting configuration (Figure 2S). Since the structural configuration of oxygen atoms surrounding a Mo site is expected to be slightly different from that associated with a V site, the structural displacements steps allowed for local structure relaxation following the swaps.

The NVT-MD annealing simulations used a time step of 0.25 fs with the temperature being controlled by a Berendsen thermostat with a temperature-damping constant of 0.05 ps. During the annealing simulation, the temperature was increased from 0 to 300K at a rate of 120 K/ps then decreased to 0 K at a slower rate of 30 K/ps except for the annealing simulations for the supercells containing vacancies, which used a constant rate of temperature change of 48 K/ps.

To prepare the slab structure from the bulk, a constrained NVT-MD simulation was employed where the c parameter was expanded from 24.03 Å to 40.00 Å at a rate of 2 Å/ps. The simulation used a time step of 0.25 fs with the temperature set at 25K and controlled by a Berendsen thermostat[5] with a temperature-damping constant of 1 fs. In addition, a center-of-mass restraint was applied to the metal atoms in each of the layers in order to maintain bulk configuration.

In order to generate the surface structure for the 6-layer slab, we started with the bulk structure and carried out ReaxFF RD while gradually stretching the c-lattice parameter to expand from the equilibrium value of 24.03 Å to 40.00 Å at a rate of 2 Å/ps. This procedure allowed ReaxFF to determine which of the interlayer metal-oxygen bonds breaks as the crystal was cleaved to form the surface, yielding the most stable locations for the interlayer oxygen atoms. The resulting slab contained 6 metal oxide layers with two (001) surfaces exposed to the propane molecules. The initial and final configurations from the ReaxFF RD simulation of the propane/Mo_3VO_x system are provided in Figure 6S.

For the ReaxFF-RD simulation of the propane/Mo_3VO_x system, we optimized the structure to minimize the energy and then performed a NVT-MD simulation with a time step of 0.15 fs with the temperature being controlled by a Berendsen thermostat[5] with a temperature-damping constant of 0.1 ps. The NVT-MD simulations of the reaction with propane were carried out for 50 ps using a dual-temperature thermostat keeping the MMO catalyst atoms were kept at 300K while the C and H atoms associated with the propane molecules were kept at 2000K. This temperature regime is maintained throughout the simulation and does not change when reactions occur. To follow the reaction events, molecular analysis of the simulations was performed using a bond order cutoff of 0.2 to allow detection of short-lived intermediates.

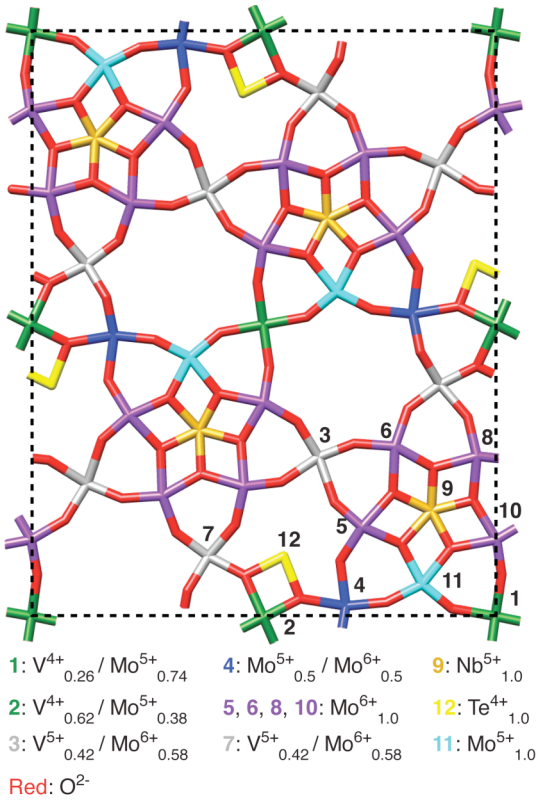

Figure 1S. Crystal structure of M1 phase of the $MoVTeNbO_x$ catalyst.

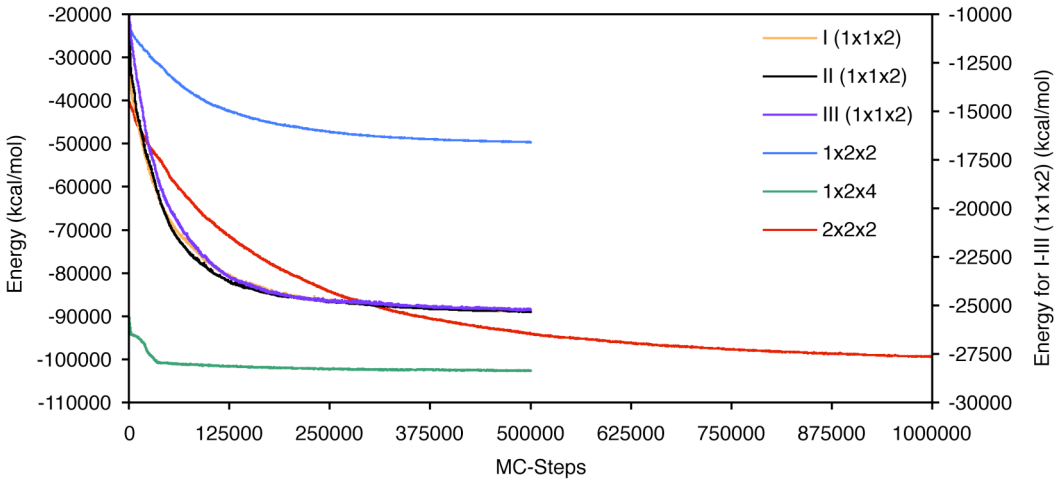

Figure 2S. ReaxFF Monte Carlo convergence for each starting configuration for the 1x1x2 supercell as well as larger supercells consisting of 1x2x2, 1x2x4, and 2x2x2.

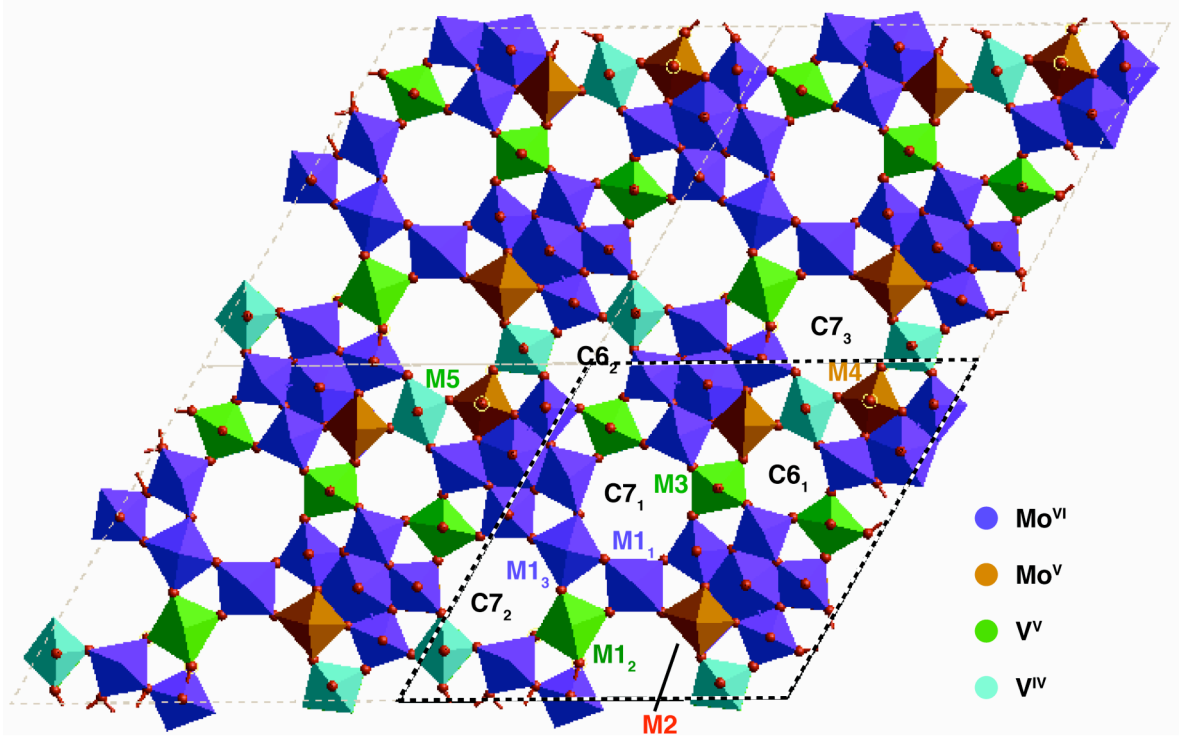

Figure 3S. Idealized polyhedra representation of the ReaxFF Mo_3VO_x structure with the oxidation states of the metals indicated by different colors (red represents oxygen). The heptagonal channel $C7_1$ contains metals in their highest oxidation state with heptagonal channels $C7_2$ and $C7_3$ containing some metals in a reduced oxidation state. In addition, hexagonal channels $C6_1$ and $C6_2$ also contain reduced metal sites.

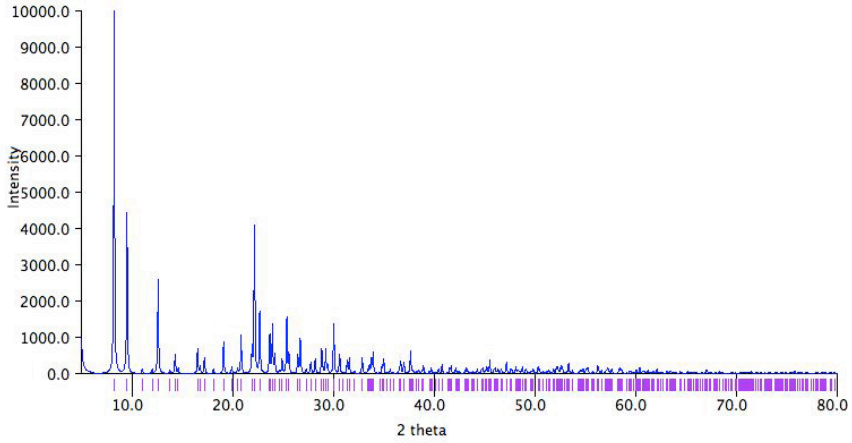

Figure 4S. Calculated x-ray powder diffraction pattern for coordinates obtained from the ReaxFF-MC-RD simulation on the 1x1x2 supercell (using Mercury[7]) employing $Cu_{K\alpha}$ radiation (λ = 1.54Å) and a symmetric pseudo-Voigt peak shape with an FWHM of 0.1° 2θ (5° > 2θ > 80°).

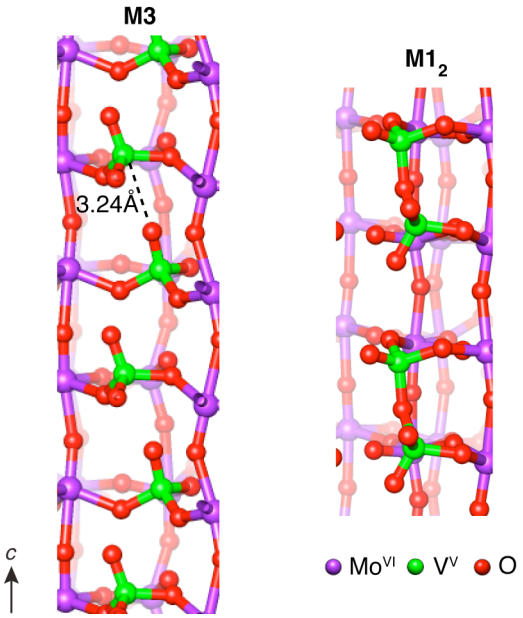

Figure 5S. Vanadium coordination for the M3 and $M1_2$ sites. In the M3 site, the vanadyl groups are aligned along the c-axis consistent with the V_2O_5 bulk structure whereas the vanadyl groups of site $M1_2$ are pointing into the $C7_2$ channel.

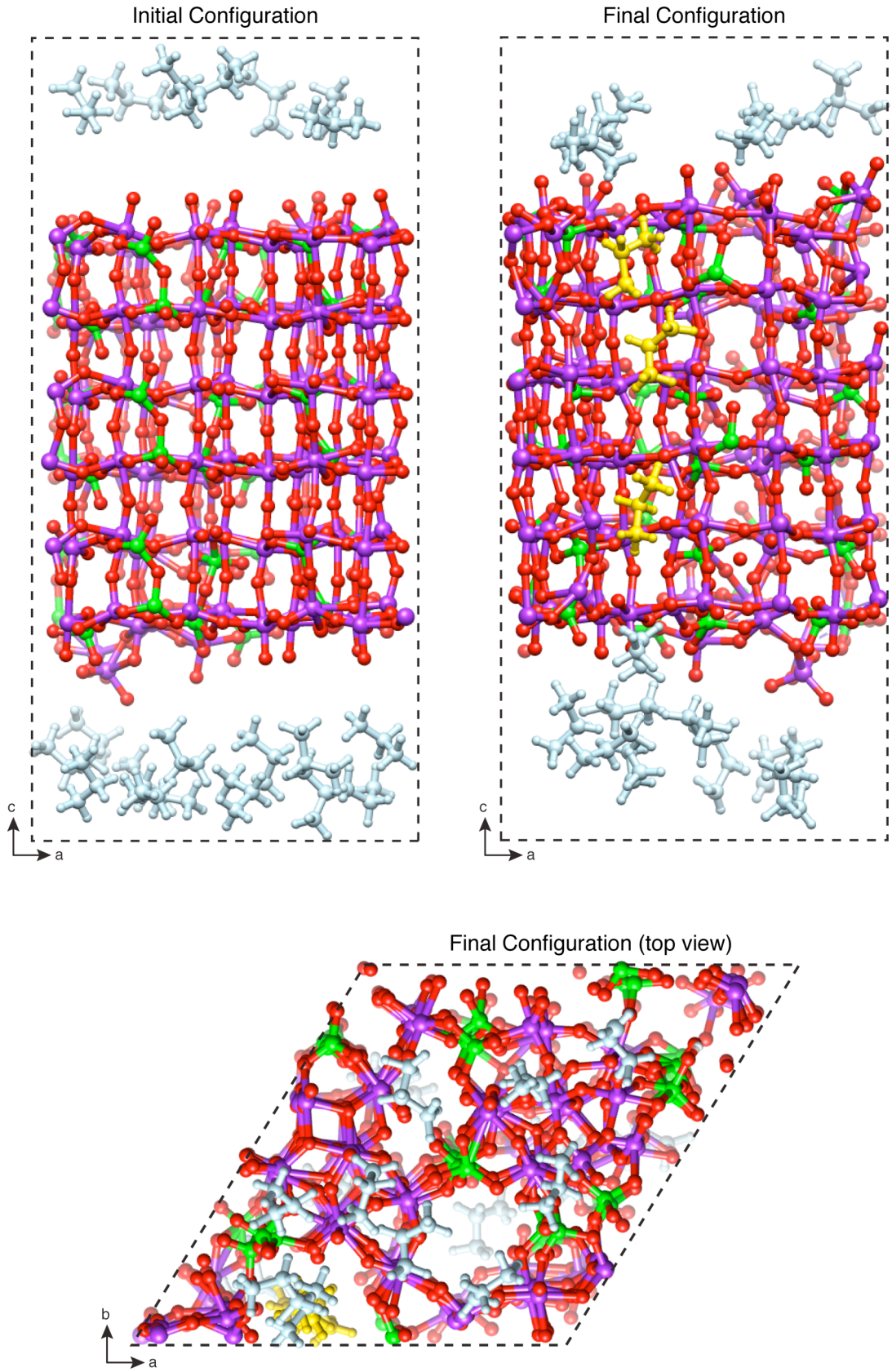

Figure 6S. Snapshots obtained from the ReaxFF-RD simulation of propane/Mo_3VO_x catalyst (Mo = purple, V = green, O = red). The propane molecules that are contained within the channel are colored yellow while the exterior propane molecules are shown in a light blue-gray.

ReaxFF Force Field Parameter File:
(This file provides the data in the format to be input into the ReaxFF program.)

```
Reactive MD-force field: c/h/o/V/Mo/Te/Nb Mo update: Feb-13-2008
 39       ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.5469 !Overcoordination parameter
   26.5405 !Valency angle conjugation parameter
    1.5105 !Triple bond stabilisation parameter
    6.6630 !Triple bond stabilisation parameter
    0.0000 !C2-correction
    1.0588 !Undercoordination parameter
    4.6000 !Triple bond stabilisation parameter
   12.1176 !Undercoordination parameter
   13.3056 !Undercoordination parameter
  -70.1292 !Triple bond stabilization energy
    0.0000 !Lower Taper-radius
   10.0000 !Upper Taper-radius
    2.8793 !Not used
   33.8667 !Valency undercoordination
    6.0891 !Valency angle/lone pair parameter
    1.0563 !Valency angle
    2.0384 !Valency angle parameter
    6.1431 !Not used
    6.9290 !Double bond/angle parameter
    0.3989 !Double bond/angle parameter: overcoord
    3.9954 !Double bond/angle parameter: overcoord
   -2.4837 !Not used
    5.7796 !Torsion/BO parameter
   10.0000 !Torsion overcoordination
    1.9487 !Torsion overcoordination
   -1.2327 !Conjugation 0 (not used)
    2.1645 !Conjugation
    1.5591 !vdWaals shielding
    0.1000 !Cutoff for bond order (*100)
    2.1365 !Valency angle conjugation parameter
    0.6991 !Overcoordination parameter
   50.0000 !Overcoordination parameter
    1.8512 !Valency/lone pair parameter
    0.5000 !Not used
   20.0000 !Not used
    5.0000 !Molecular energy (not used)
    0.0000 !Molecular energy (not used)
    2.6962 !Valency angle conjugation parameter
  8    ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
           alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
           cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
           ov/un;val1;n.u.;val3,vval4
 C     1.3825   4.0000  12.0000   1.9133   0.1853   0.9000   1.1359   4.0000
       9.7602   2.1346   4.0000  33.2433  79.5548   5.8678   7.0000   0.0000
       1.2104   0.0000 199.0303   8.6991  34.7289  13.3894   0.8563   0.0000
      -2.8983   2.5000   1.0564   4.0000   2.9663   0.0000   0.0000   0.0000
 H     0.7853   1.0000   1.0080   1.5904   0.0419   1.0206  -0.1000   1.0000
       9.3557   5.0518   1.0000   0.0000 121.1250   5.3200   7.4366   1.0000
      -0.1000   0.0000  62.4879   1.9771   3.3517   0.7571   1.0698   0.0000
     -15.7683   2.1488   1.0338   1.0000   2.8793   0.0000   0.0000   0.0000
 O     1.2477   2.0000  15.9990   1.9236   0.0904   1.0503   1.0863   6.0000
      10.2127   7.7719   4.0000  36.9573 116.0768   8.5000   8.9989   2.0000
       0.9088   1.0003  60.8726  20.4140   3.3754   0.2702   0.9745   0.0000
      -3.6141   2.7025   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
 V     2.3008   3.0000  50.9415   1.8842   0.2471   0.5518   0.1000   5.0000
      12.3750   5.2538   3.0000   0.0000   0.0000   2.1056   5.4975   0.0000
      -1.0000   0.0000 117.6300  23.2444   6.5966   1.0000   0.8563   0.0000
      -3.2973   2.3344   1.0338   6.0000   3.6411   0.0000   0.0000   0.0000
 Mo    2.4710   5.6504  95.9400   1.8000   0.3285   1.0000   0.1000   6.0000
```

```
    13.0000  45.0000   4.0000   0.0000   0.0000   0.6062   6.1484   0.0000
     0.1000   0.0000 152.6300   3.7659   0.0689   2.9902   0.8563   0.0000
   -16.7660   3.1072   1.0338   8.0000   3.4590   0.0000   0.0000   0.0000
Te   2.2837   2.0000 127.6004   2.0843   0.3994   1.0000   0.0535   6.0000
    10.9769  14.9210   4.0000   0.0001   0.0000   0.5335   5.5000   0.0000
    -1.0000  31.9710  50.0000  24.8446   1.6557   0.1542   0.8563   0.0000
    -4.9158   2.6995   1.0338   6.0000   2.5791   0.0000   0.0000   0.0000
Nb   1.9727   3.0000  92.9064   2.9000   0.0622   0.5561   0.1000   5.0000
    11.6835   1.0000   3.0000   0.0000   0.0000   0.8579   5.5059   0.0000
    -1.0000   0.0000 117.6300  23.5591   6.7940   1.0000   0.8563   0.0000
    -4.9213   2.3925   1.0338   6.0000   3.6411   0.0000   0.0000   0.0000
X   -0.1000   2.0000   1.0080   2.0000   0.0000   1.0000  -0.1000   6.0000
    10.0000   2.5000   4.0000   0.0000   0.0000   8.5000   1.5000   0.0000
    -0.1000   0.0000  -2.3700   8.7410  13.3640   0.6690   0.9745   0.0000
   -11.0000   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
30      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                       pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
 1  1 156.5953 100.0397  80.0000  -0.8157  -0.4591   1.0000  37.7369   0.4235
        0.4527  -0.1000   9.2605   1.0000  -0.0750   6.8316   1.0000   0.0000
 1  2 170.2316   0.0000   0.0000  -0.5931   0.0000   1.0000   6.0000   0.7140
        5.2267   1.0000   0.0000   1.0000  -0.0500   6.8315   0.0000   0.0000
 2  2 156.0973   0.0000   0.0000  -0.1377   0.0000   1.0000   6.0000   0.8240
        2.9907   1.0000   0.0000   1.0000  -0.0593   4.8358   0.0000   0.0000
 1  3 160.4802 105.1693  23.3059  -0.3873  -0.1613   1.0000  10.8851   1.0000
        0.5341  -0.3174   7.0303   1.0000  -0.1463   5.2913   0.0000   0.0000
 3  3  60.1463 176.6202  51.1430  -0.2802  -0.1244   1.0000  29.6439   0.9114
        0.2441  -0.1239   7.6487   1.0000  -0.1302   6.2919   1.0000   0.0000
 4  4  36.0707   0.0000   0.0000   0.1764  -0.3000   0.0000  16.0000   0.1020
        0.0350  -0.3000  16.0000   1.0000  -0.0587   8.4813   0.0000   0.0000
 3  4 137.8828  56.4570   0.0000   0.0310  -0.3000   1.0000  36.0000   0.2355
        0.7943  -0.2977  15.9401   1.0000  -0.1952   5.0015   1.0000   0.0000
 2  4 112.6739   0.0000   0.0000   0.1669  -0.3000   0.0000  36.0000   0.0751
       -0.4510  -0.2500  20.0000   1.0000  -0.0822   6.4179   0.0000   0.0000
 1  4 130.2004   0.0000   0.0000  -0.3153  -0.3000   1.0000  36.0000   0.6315
        0.9750  -0.2500  20.0000   1.0000  -0.1203   6.5055   1.0000   0.0000
 1  5   0.5356   0.9614   0.0000   0.3817  -0.3000   1.0000  36.0000   0.2142
        0.6116  -0.2579   6.1366   1.0000  -0.0913   6.6008   1.0000   0.0000
 2  5   0.0000   0.0000   0.0000  -0.2872  -0.3000   1.0000  36.0000   0.0082
        1.7973  -0.3027   4.6243   1.0000  -0.4578   3.5219   1.0000   0.0000
 3  5 113.2223  29.8045  86.9949   0.4438  -0.2465   1.0000  16.6234   1.0764
        0.1199  -0.1696   7.0000   1.0000  -0.1734   5.4732   1.0000   0.0000
 5  5  44.7260   0.0000   0.0000   1.0000  -0.3000   0.0000  16.0000   0.2910
        0.3462  -0.3000  16.0000   1.0000  -0.1862   7.4588   0.0000   0.0000
 1  6   0.0000   0.0000   0.0000   0.5000  -0.2000   0.0000  16.0000   0.5000
        0.5000  -0.2000  15.0000   1.0000  -0.2000  15.0000   0.0000   0.0000
 2  6   0.0000   0.0000   0.0000   0.5000  -0.2000   0.0000  16.0000   0.5000
        0.5000  -0.2000  15.0000   1.0000  -0.2000  15.0000   0.0000   0.0000
 3  6 145.3033 108.2699   0.0000  -1.0000  -0.2000   1.0000  16.0000   0.1058
        0.9966  -0.3500  12.3131   1.0000  -0.1995   5.4880   1.0000   0.0000
 6  6  87.6524   0.0000   0.0000  -0.7892  -0.2000   0.0000  16.0000   0.7157
        0.9313  -0.2000  12.0000   1.0000  -0.1500   6.6119   0.0000   0.0000
 7  7  69.7508   0.0000   0.0000   1.0000  -0.3000   0.0000  16.0000   0.3527
        0.5402  -0.3000  16.0000   1.0000  -0.0723   5.6715   0.0000   0.0000
 3  7 172.1593  81.6477   0.0000   0.0680  -0.3000   1.0000  36.0000   0.1000
        0.6829  -0.2981  15.8837   1.0000  -0.1898   4.5690   1.0000   0.0000
 1  7   0.0000   0.0000   0.0000  -0.2872  -0.3000   1.0000  36.0000   0.0082
        1.7973  -0.2500  20.0000   1.0000  -0.2578   6.5219   1.0000   0.0000
 2  7   0.0000   0.0000   0.0000  -0.2872  -0.3000   1.0000  36.0000   0.0082
        1.7973  -0.2500  20.0000   1.0000  -0.2578   6.5219   1.0000   0.0000
 4  5  52.9011   0.0000   0.0000  -0.5114  -0.3000   0.0000  16.0000   0.3099
        0.3693  -0.3000  16.0000   1.0000  -0.0571   8.7632   0.0000   0.0000
12  5  59.6440   0.0000   0.0000  -0.9780  -0.3000   0.0000  16.0000   0.3138
        1.2787  -0.3000  16.0000   1.0000  -0.0599   6.2819   0.0000   0.0000
 4  6 102.9033   0.0000   0.0000  -1.0000  -0.3000   0.0000  16.0000   0.3130
        0.7191  -0.3000  16.0000   1.0000  -0.0797   5.6372   0.0000   0.0000
```

```
12  6   0.0000   0.0000   0.0000  -0.5000  -0.2000   0.0000  16.0000   0.5000
        0.2500  -0.2000  12.0000   1.0000  -0.2500  12.0000   0.0000   0.0000
 5  6  95.7732   0.0000   0.0000  -1.0000  -0.3000   0.0000  16.0000   0.3208
        1.3541  -0.3000  16.0000   1.0000  -0.0779   5.6686   0.0000   0.0000
 4  7  69.5784   0.0000   0.0000   0.2297  -0.3000   0.0000  16.0000   0.3021
        2.0000  -0.3000  16.0000   1.0000  -0.1081   6.1251   0.0000   0.0000
12  7   0.0000   0.0000   0.0000  -0.5000  -0.2000   0.0000  16.0000   0.5000
        0.2500  -0.2000  12.0000   1.0000  -0.2500  12.0000   0.0000   0.0000
 5  7 104.9927   0.0000   0.0000  -0.6232  -0.3000   0.0000  16.0000   0.3000
        1.1567  -0.3000  16.0000   1.0000  -0.0998   5.8400   0.0000   0.0000
 6  7   0.0000   0.0000   0.0000  -0.5000  -0.2000   0.0000  16.0000   0.5000
        0.2500  -0.2000  12.0000   1.0000  -0.2500  12.0000   0.0000   0.0000
13    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2   0.1219   1.4000   9.8442   1.1203  -1.0000  -1.0000
 2  3   0.0344   1.6800  10.3247   0.9013  -1.0000  -1.0000
 1  3   0.1131   1.8523   9.8442   1.2775   1.1342   1.0621
 1  4   0.1005   1.7015  12.0291   1.8429  -1.0000  -1.0000
 2  4   0.1211   1.6565  10.7328   1.4538  -1.0000  -1.0000
 3  4   0.0807   1.9659  10.0132   1.6500   1.5900  -1.0000
 1  5   0.1495   2.0794  12.2376   0.0100   1.4060  -1.0000
 2  5   0.0795   1.6794  11.2376   0.0100   1.2060  -1.0000
 3  5   0.1453   1.8849  10.8505   1.6926   1.5319   1.6459
 3  6   0.4351   1.8000  10.9741   1.9974   1.7134  -1.0000
 1  7   0.0967   1.5551  11.8614   1.7533   1.0288  -1.0000
 2  7   0.2255   1.8441  10.7044   1.6296   1.0434  -1.0000
 3  7   0.2305   1.9793  10.3634   1.7902   1.7143  -1.0000
56    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
 1  1  1  67.2326  22.0695   1.6286   0.0000   1.7959  15.4141   1.8089
 1  1  2  65.2527  14.3185   6.2977   0.0000   0.5645   0.0000   1.1530
 2  1  2  70.0840  25.3540   3.4508   0.0000   0.0050   0.0000   3.0000
 1  2  2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000   1.0400
 1  2  1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000   1.0400
 2  2  2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000   1.0400
 1  1  3  49.5561   7.3771   4.9568   0.0000   0.7533  15.9906   1.0010
 3  1  3  77.1171  39.8746   2.5403 -24.3902   1.7740 -42.9758   2.1240
 2  1  3  65.0000  14.2057   4.8649   0.0000   0.3504   0.0000   1.7185
 1  3  1  74.3994  44.7500   0.7982   0.0000   3.0000   0.0000   1.0528
 1  3  3  77.9854  36.6201   2.0201   0.0000   0.7434  67.0264   3.0000
 3  3  3  80.7324  30.4554   0.9953   0.0000   1.6310  50.0000   1.0783
 1  3  2  71.5018  21.7062   0.4735   0.0000   0.5186   0.0000   1.1793
 2  3  3  84.9468  23.3540   1.5057   0.0000   2.6374   0.0000   1.3023
 2  3  2  77.0645  10.4737   1.2895   0.0000   0.9924   0.0000   1.1043
 1  2  3   0.0000   5.0000   3.0000   0.0000   1.0000   0.0000   1.5000
 3  2  3   0.0000   0.0148   6.0000   0.0000   0.0000   0.0000   1.0400
 2  2  3   0.0000   9.7025   6.0000   0.0000   0.0000   0.0000   1.0400
 3  4  3  68.9780  25.4118   1.8941   0.0000   2.6245   0.0000   1.0010
 4  3  4  57.5689   6.3911   5.0236   0.0000   1.0358   0.0000   2.5634
 3  3  4  54.0069   6.0419   1.1089   0.0000   2.7213   0.0000   2.4129
 1  3  4  67.7243   5.1160   5.6779   0.0000   1.0536   0.0000   1.0010
 2  3  4 100.0000  12.7432   1.5773   0.0000   1.3885   0.0000   3.8809
 3  4  4  22.6212   4.2523   3.3011   0.0000   1.1185   0.0000   2.2035
 3  5  3  83.1357  10.0000   3.5278   0.0000   3.5962   0.0000   2.2128
 5  3  5  42.8017  15.2673   0.2124   0.0000   3.9192   0.0000   1.9629
 3  3  5   5.0000   1.1358   5.7500   0.0000   0.7307   0.0000   1.0500
 3  5  5  87.6269  13.4392   0.3503   0.0000   3.7497   0.0000   1.9735
 2  3  5  89.5346   8.1714   5.1415   0.0000   1.5293   0.0000   1.0500
 1  3  5 100.0000   5.5890   6.0000   0.0000   2.0169   0.0000   4.0000
 1  1  4  70.0000  14.3983   2.0000   0.0000   1.0000   0.0000   1.2000
 2  1  4  70.0000   7.0700   2.0000   0.0000   1.0000   0.0000   1.2000
 3  1  4  70.8486  39.9493   1.8219   0.0000   1.0000   0.0000   1.1696
 1  2  4   0.0000   5.0000   2.0000   0.0000   1.0000   0.0000   1.2000
 2  2  4   0.0000   9.0000   2.0000   0.0000   1.0000   0.0000   1.2000
 3  2  4   0.0000   5.9843   1.8885   0.0000   1.0000   0.0000   1.2456
 1  4  1  70.0000  23.6766   1.0000   0.0000   1.0000   0.0000   1.2000
 1  4  2  70.0000   6.0546   1.0000   0.0000   1.0000   0.0000   1.2000
```

```
 1  4  3  64.7486  23.1702   3.0204   0.0000   1.0000   0.0000   1.0937
 2  4  2  65.0000  11.6200   1.0000   0.0000   1.0000   0.0000   1.2000
 2  4  3  60.4260  22.5101   3.6090   0.0000   1.0000   0.0000   1.2953
 6  6  6  43.4601   0.1547  10.0000   0.0000   3.0000   0.0000   4.0000
 3  6  3  89.7270  17.6782   6.0893   0.0000   0.1224   0.0000   1.0010
 6  3  6 100.0000   9.4130   7.0000   0.0000   2.9820   0.0000   1.0010
 3  3  6  86.1101  37.8909   6.8533   0.0000   2.3084   0.0000   1.0010
 2  3  6  88.7352   6.5059   5.8319   0.0000   0.1581   0.0000   1.3712
 1  3  6  62.5875   9.3785   2.7541   0.0000   0.8214   0.0000   1.0010
 3  7  3  78.3215  28.6208   2.2037   0.0000   2.8954   0.0000   1.0010
 7  3  7  11.2811  33.8842   0.6392   0.0000   1.6448   0.0000   1.0010
 3  3  7  48.4192  18.2610   6.2579   0.0000   3.0000   0.0000   1.0010
 1  3  7  38.5678  10.2521   0.4517   0.0000   1.0140   0.0000   3.0000
 2  3  7 100.0000  17.5579   7.0000   0.0000   0.2673   0.0000   3.9784
 4  3  5  73.3964  11.0629   1.4212   0.0000   1.3131   0.0000   1.1514
 4  3  6  73.7648   4.0000   6.7042   0.0000   1.0000   0.0000   1.0010
 5  3  6  67.4241  14.0739   2.1553   0.0000   1.5695   0.0000   1.5000
 5  3  7  45.2045   5.5907   1.4635   0.0000   2.1119   0.0000   1.3069
36    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1  1  1  1  -0.2500  11.5822   0.1879  -4.7057  -2.2047   0.0000   0.0000
 1  1  1  2  -0.2500  31.2596   0.1709  -4.6391  -1.9002   0.0000   0.0000
 2  1  1  2  -0.1770  30.0252   0.4340  -5.0019  -2.0697   0.0000   0.0000
 1  1  1  3  -0.7098  22.2951   0.0060  -2.5000  -2.1688   0.0000   0.0000
 2  1  1  3  -0.3568  22.6472   0.6045  -4.0088  -1.0000   0.0000   0.0000
 3  1  1  3  -0.0528   6.8150   0.7498  -5.0913  -1.0000   0.0000   0.0000
 1  1  3  1   2.0007  25.5641  -0.0608  -2.6456  -1.1766   0.0000   0.0000
 1  1  3  2  -1.1953  42.1545  -1.0000  -8.0821  -1.0000   0.0000   0.0000
 2  1  3  1  -0.9284  34.3952   0.7285  -2.5440  -2.4641   0.0000   0.0000
 2  1  3  2  -2.5000  79.6980   1.0000  -3.5697  -2.7501   0.0000   0.0000
 1  1  3  3  -0.0179   5.0603  -0.1894  -2.5000  -2.0399   0.0000   0.0000
 2  1  3  3  -0.5583  80.0000   1.0000  -4.4000  -3.0000   0.0000   0.0000
 3  1  3  1  -2.5000  76.0427  -0.0141  -3.7586  -2.9000   0.0000   0.0000
 3  1  3  2   0.0345  78.9586  -0.6810  -4.1777  -3.0000   0.0000   0.0000
 3  1  3  3  -2.5000  66.3525   0.3986  -3.0293  -3.0000   0.0000   0.0000
 1  3  3  1   2.5000  -0.5332   1.0000  -3.5096  -2.9000   0.0000   0.0000
 1  3  3  2  -2.5000   3.3219   0.7180  -5.2021  -2.9330   0.0000   0.0000
 2  3  3  2   2.2500  -6.2288   1.0000  -2.6189  -1.0000   0.0000   0.0000
 1  3  3  3   0.0531 -17.3983   1.0000  -2.5000  -2.1584   0.0000   0.0000
 2  3  3  3   0.4723 -12.4144  -1.0000  -2.5000  -1.0000   0.0000   0.0000
 3  3  3  3  -2.5000 -25.0000   1.0000  -2.5000  -1.0000   0.0000   0.0000
 0  1  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  2  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  1  1  0   0.0000  50.0000   0.3000  -4.0000  -2.0000   0.0000   0.0000
 0  3  3  0   0.5511  25.4150   1.1330  -5.1903  -1.0000   0.0000   0.0000
 2  1  3  5   0.3132  10.0000   0.1000  -9.0000  -2.1000   0.0000   0.0000
 1  1  3  5   2.5000  10.0000   0.1000  -9.0000  -2.1000   0.0000   0.0000
 2  3  5  3   2.0268  10.0000   1.0000  -9.0000  -1.0000   0.0000   0.0000
 2  3  4  3   0.6439  21.4220  -0.6344  -5.5022   0.0000   0.0000   0.0000
 1  3  4  3  -0.5000  26.4579  -1.0000  -6.1063   0.0000   0.0000   0.0000
 1  1  3  4  -0.5000   5.9300  -1.0000  -6.1328   0.0000   0.0000   0.0000
 2  1  3  4   1.5000  13.6826   0.1478  -2.9478   0.0000   0.0000   0.0000
 4  3  3  4  -0.0641  59.7588  -1.0000  -3.5975   0.0000   0.0000   0.0000
 3  3  4  3   1.5000  51.9995   0.4171  -2.5000   0.0000   0.0000   0.0000
 4  3  4  3   0.0000   0.0000   0.0000  -9.0000   0.0000   0.0000   0.0000
 1    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
 3  2  3   2.1082  -2.5000   3.0000  23.0000
```